LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051821\
Data File : VN067129.D
Acq On : 18 May 2021 16:03
Operator : JC/MD
Sample : M2387-08
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 41801

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051421W.M
Title : SW846 8260

Signal : TIC: VN067129.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.820	19	30	51	rVB	169691	250403	9.13%	1.405%
2	2.152	144	154	173	rBV3	54916	102500	3.74%	0.575%
3	3.654	698	714	733	rBV2	15810	39580	1.44%	0.222%
4	3.772	741	758	782	rVB2	24836	67351	2.45%	0.378%
5	4.757	1084	1125	1163	rBV5	37323	192629	7.02%	1.081%
6	5.872	1512	1541	1573	rBV2	298932	1092193	39.80%	6.129%
7	6.465	1739	1762	1792	rBV4	140476	443934	16.18%	2.491%
8	6.760	1854	1872	1897	rBV2	24696	76590	2.79%	0.430%
9	7.130	1991	2010	2025	rBV2	16382	48329	1.76%	0.271%
10	7.519	2134	2155	2169	rBV2	363420	929585	33.88%	5.217%
11	7.597	2170	2184	2213	rVB2	676250	1647228	60.03%	9.244%
12	7.962	2297	2320	2347	rBV2	400483	1026996	37.43%	5.763%
13	8.203	2391	2410	2432	rVB4	50820	119594	4.36%	0.671%
14	8.525	2510	2530	2564	rBV	885311	1914335	69.77%	10.743%
15	9.077	2723	2736	2775	rVB5	47424	123593	4.50%	0.694%
16	10.037	3073	3094	3109	rBV	1471528	2743974	100.00%	15.399%
17	10.102	3109	3118	3149	rVB	160705	324008	11.81%	1.818%
18	11.360	3569	3587	3617	rBV	1079233	2055000	74.89%	11.532%
19	11.577	3655	3668	3696	rBV2	47429	124282	4.53%	0.697%
20	11.907	3779	3791	3812	rBV2	23068	55123	2.01%	0.309%
21	12.360	3943	3960	4014	rBV	747933	1728745	63.00%	9.702%
22	12.794	4108	4122	4124	rBV9	23285	34419	1.25%	0.193%
23	13.001	4190	4199	4211	rVB2	30578	48431	1.76%	0.272%
24	13.071	4212	4225	4247	rBV2	116522	285239	10.40%	1.601%
25	13.154	4249	4256	4267	rVB2	50447	72791	2.65%	0.408%
26	13.299	4296	4310	4342	rBV	827694	1718166	62.62%	9.642%
27	13.419	4344	4355	4412	rVB	152435	554243	20.20%	3.110%

Sum of corrected areas: 17819261

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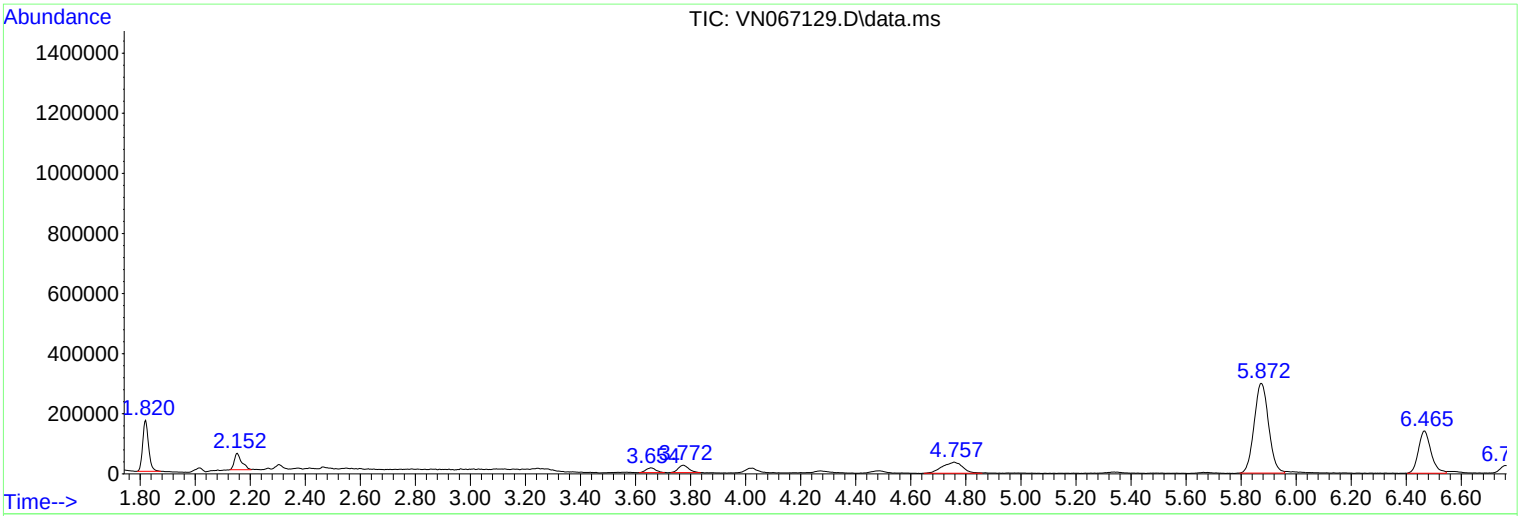
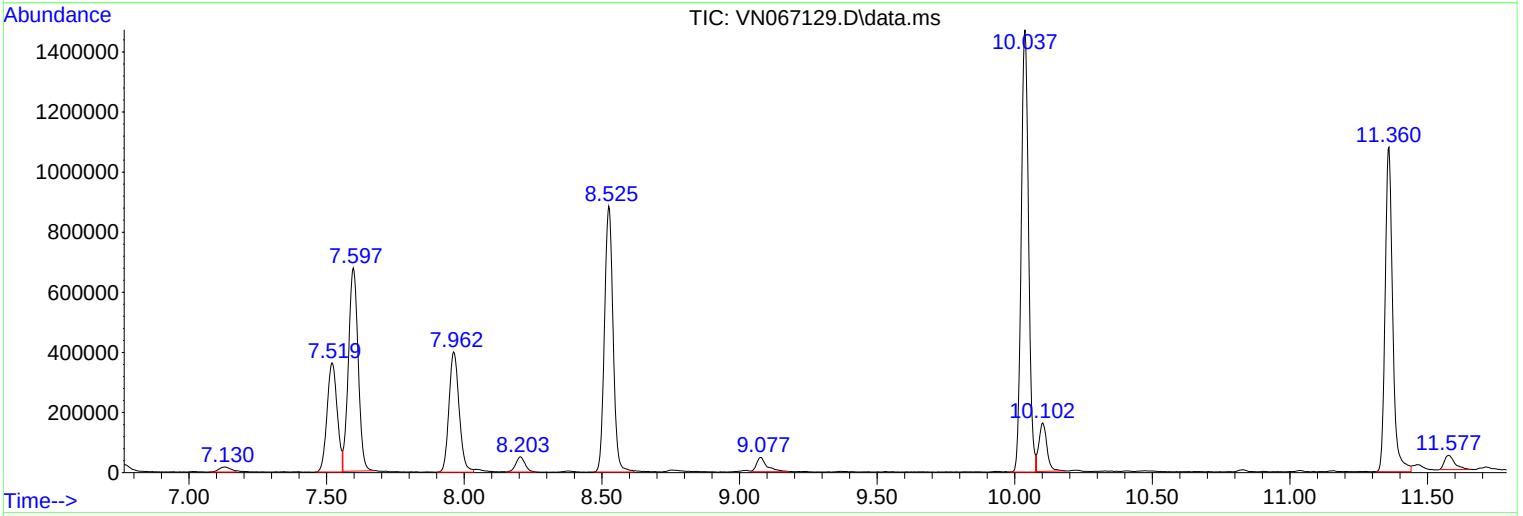
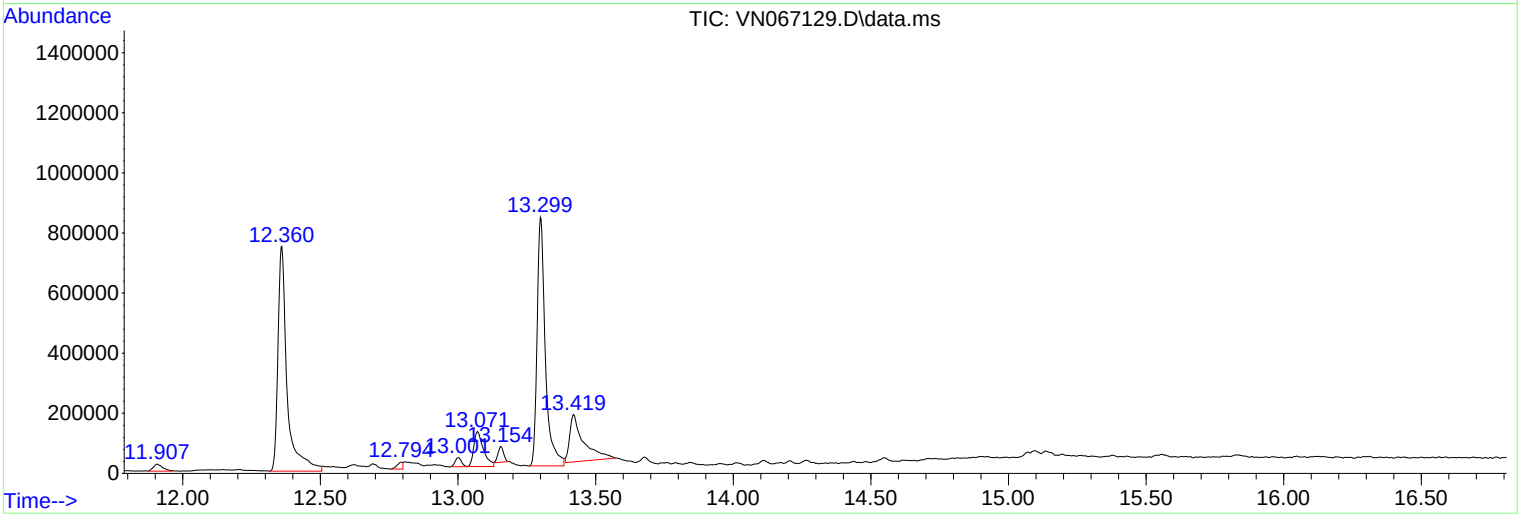
Instrument :
MSVOA_N
ClientSampleId :
41801

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P







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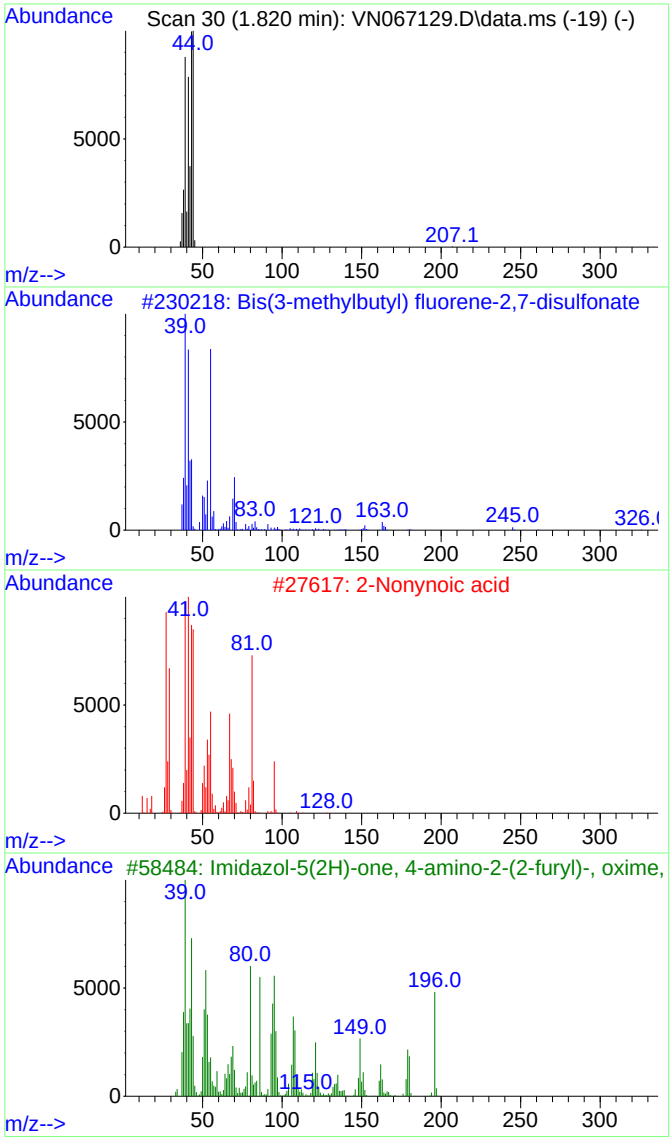
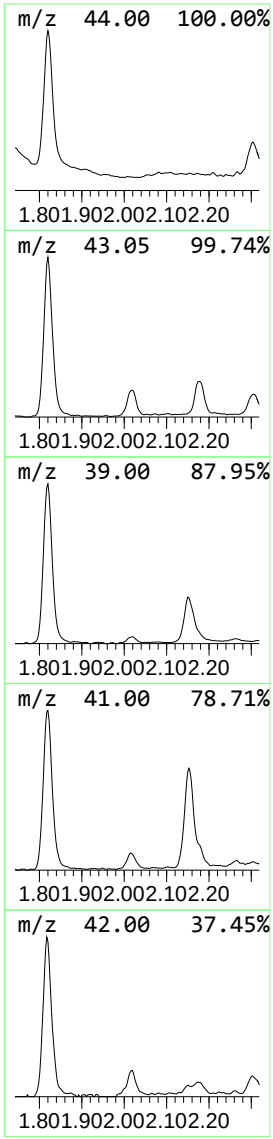
****
Peak Number 1 Bis(3-methylbutyl) fluorene... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.820	7.60 ug/l	250403	Pentafluorobenzene	7.597

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bis(3-methylbutyl) fluorene-2,7-...	466	C23H30O6S2	253664-95-8	64
2	2-Nonynoic acid	154	C9H14O2	001846-70-4	45
3	Imidazol-5(2H)-one, 4-amino-2-(2...	196	C7H8N4O3	318259-17-5	45
4	Cyclopropanecarboxamide	85	C4H7NO	006228-73-5	43
5	2-Hexynoic acid	112	C6H8O2	000764-33-0	43





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Instrument : MSVOA_N
ClientSampleId : 41801

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Quant Title : SW846 8260

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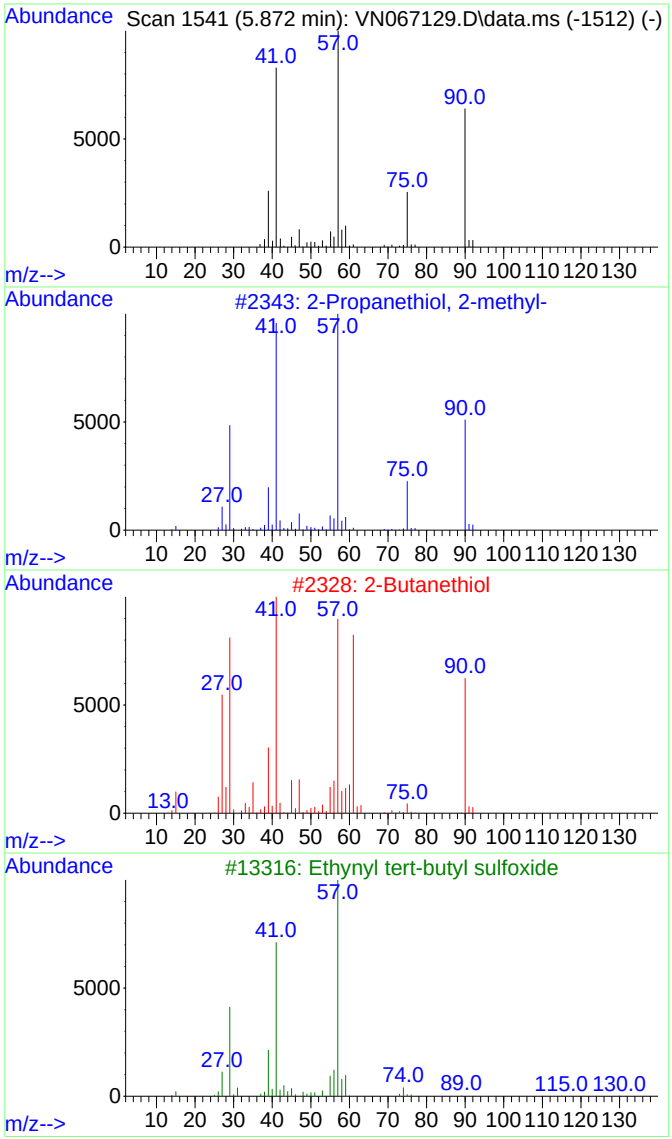
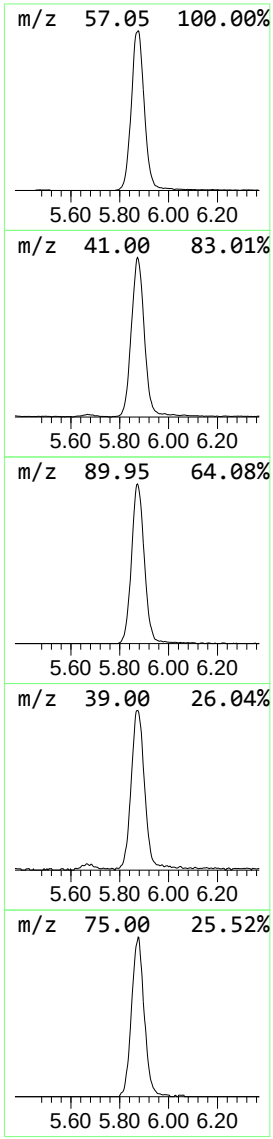
****
Peak Number 2 2-Propanethiol, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.872	33.15 ug/l	1092190	Pentafluorobenzene	7.597

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanethiol, 2-methyl-	90	C4H10S	000075-66-1	91
2	2-Butanethiol	90	C4H10S	000513-53-1	42
3	Ethynyl tert-butyl sulfoxide	130	C6H10OS	041463-34-7	16
4	Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	14
5	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	14





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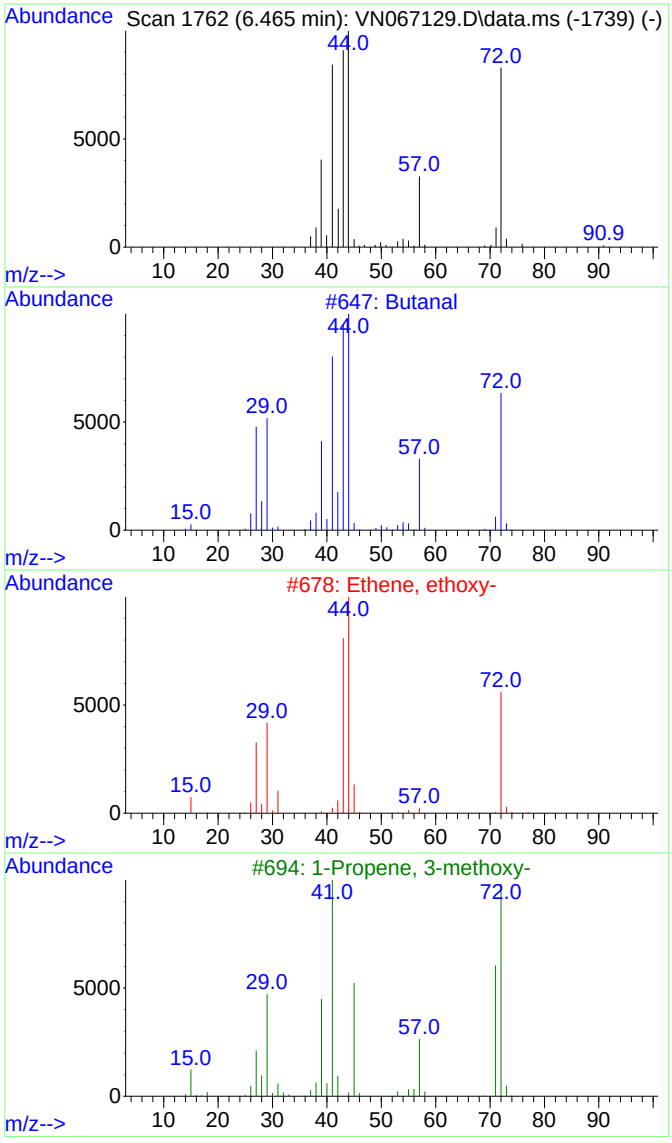
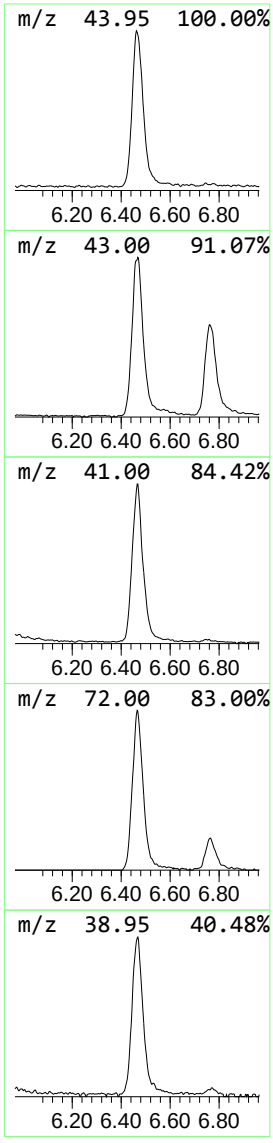
****

Peak Number 3 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.465	13.48 ug/l	443934	Pentafluorobenzene	7.597

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	94
2	Ethene, ethoxy-	72	C4H8O	000109-92-2	53
3	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	43
4	Propanal, 2-methyl-	72	C4H8O	000078-84-2	38
5	Isobutylene epoxide	72	C4H8O	000558-30-5	27





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Instrument : MSVOA_N
ClientSampleId : 41801

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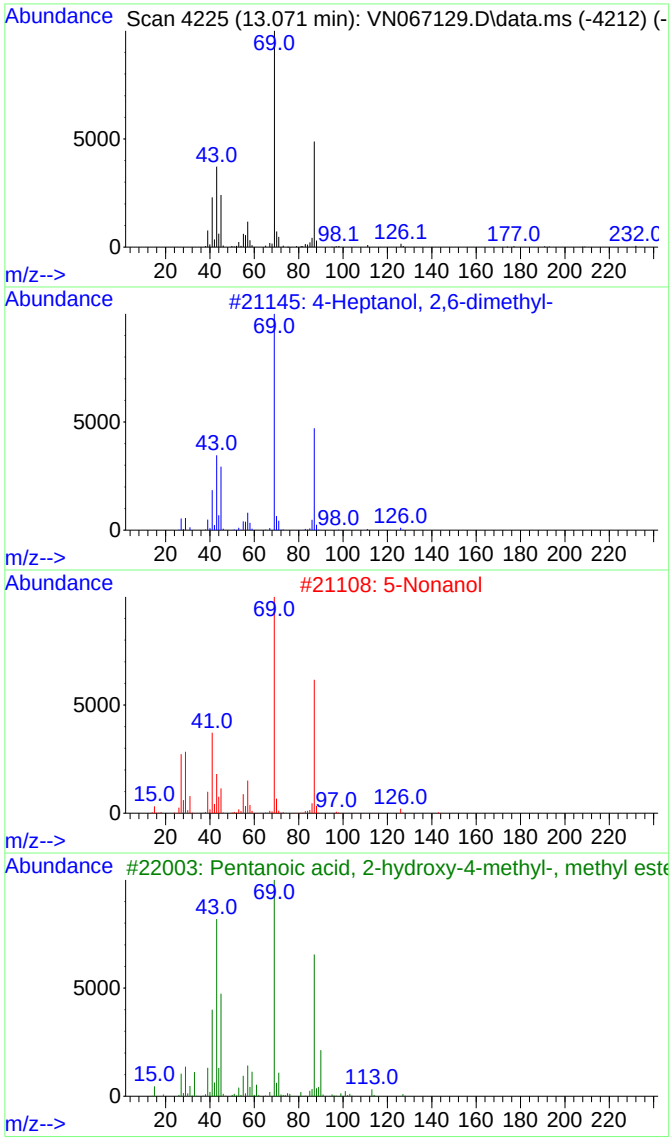
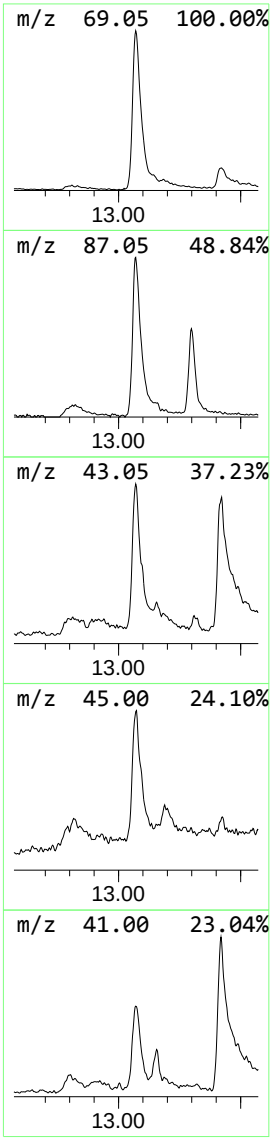
****
Peak Number 4 4-Heptanol, 2,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.071	8.30 ug/l	285239	1,4-Dichlorobenzene-d4	13.301

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol, 2,6-dimethyl-	144	C9H20O	000108-82-7	90
2	5-Nonanol	144	C9H20O	000623-93-8	86
3	Pentanoic acid, 2-hydroxy-4-meth...	146	C7H14O3	040348-72-9	78
4	Ethyl dl-2-hydroxycaproate	160	C8H16O3	006946-90-3	74
5	1,2-Hexanediol	118	C6H14O2	006920-22-5	72





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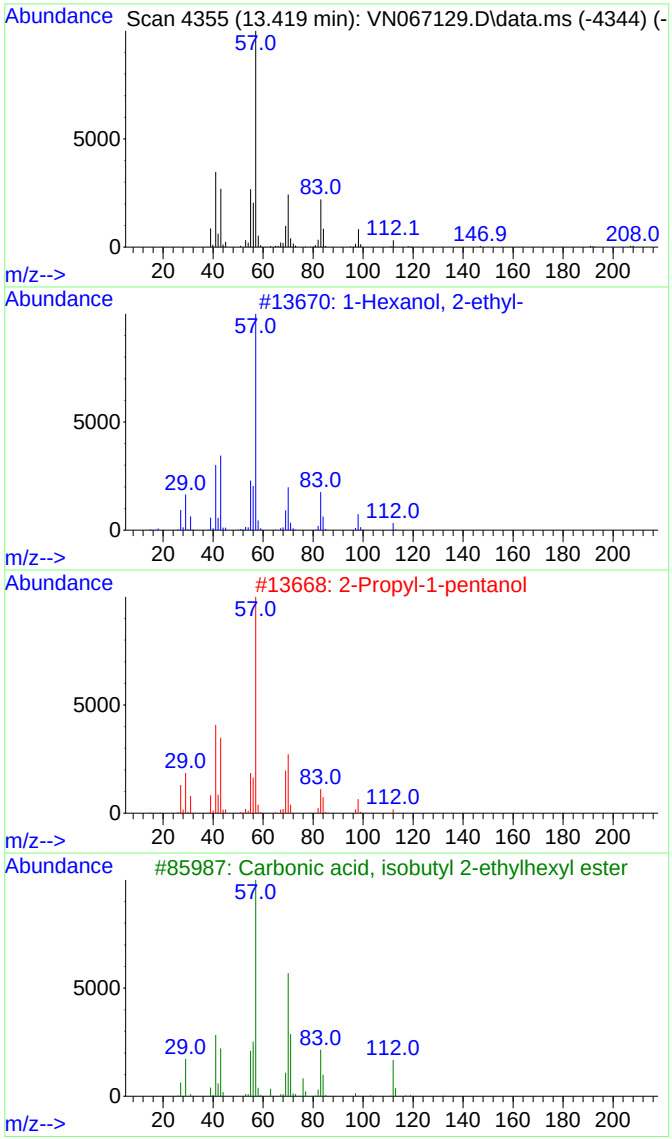
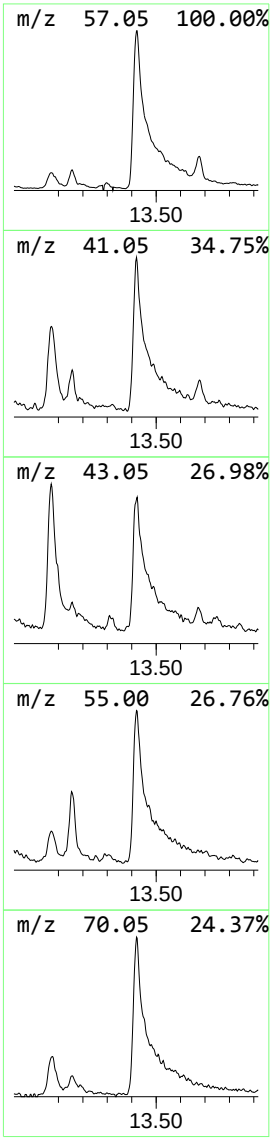
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.419	16.13 ug/l	554243	1,4-Dichlorobenzene-d4	13.301

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59
3	Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000357-82-9	53
4	Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	53
5	2-Ethyl-1-hexanol, pentafluoropr...	276	C11H17F5O2	1000365-51-1	47





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Bis(3-methylbut...	1.820	7.6	ug/l	250403	1	7.597	1647230	50.0
2-Propanethiol,...	5.872	33.1	ug/l	1092190	1	7.597	1647230	50.0
Butanal	6.465	13.5	ug/l	443934	1	7.597	1647230	50.0
4-Heptanol, 2,6...	13.071	8.3	ug/l	285239	4	13.301	1718170	50.0
1-Hexanol, 2-et...	13.419	16.1	ug/l	554243	4	13.301	1718170	50.0